

WHAT IS CLAIMED IS:

1. A computer-implemented method for generating a library design for a set of experiments, comprising:

defining a library array representing an arrangement of experiments in the set of experiments, the library array including electronic data defining a plurality of elements, each of the plurality of elements representing a potential location for an experiment in the set of experiments;

defining a plurality of sources, each of the plurality of sources including electronic data representing a material or condition that can be used in the set of experiments;

receiving user input defining a plurality of maps representing the application of sources to elements of the library array, each of the plurality of maps including electronic data identifying one or more library elements and defining an amount of a corresponding source to be applied to the identified library elements, the plurality of maps being ordered to define a mapping sequence; and

generating a library design including electronic data representing the library array, the sources, the maps and the mapping sequence, the library design specifying for each of a plurality of library elements amounts of one or more sources to be applied to the corresponding library element, the amounts being defined at least in part by the order of maps in the mapping sequence.

2. The method of claim 1, further comprising:

displaying a visual representation of a plurality of experiments in the set of experiments.

3. The method of claim 2, wherein:

the visual representation includes a representation of at least a portion of composition including the specified amounts for a plurality of library elements corresponding to the plurality of experiments.

4. The method of claim 2, wherein:

the visual representation includes a representation of the mapping sequence, the maps in the mapping sequence being selectable in the visual representation.

5. The method of claim 4, wherein:

the visual representation includes a representation of a portion of a composition including the specified amounts for a plurality of library elements, the portion being determined based on a set of maps selected by the user.

6. The method of claim 1, wherein:

one or more of the maps in the mapping sequence has an associated equation defining a mathematical relationship for determining the amount of the corresponding source to be applied to the identified library elements based on an amount defined by a prior map in the mapping sequence.

7. The method of claim 6, wherein:

the mapping sequence includes a first group of maps, the first group of maps having a first set of associated equations defining a plurality of mathematical relationships for determining the amount of one or more sources to be applied to one or more identified library elements, the first set of associated equations being solvable as a set of simultaneous equations.

8. The method of claim 7, wherein:

the mapping sequence includes a second group of maps, the second group of maps having a second set of associated equations defining a plurality of mathematical relationships for determining the amount of one or more sources to be applied to one or more identified library elements, the first set of associated equations and second set of associated equations being separately solvable as sets of simultaneous equations.

9. The method of claim 1, wherein:

the plurality of maps includes a remove map defining an amount of a source to be removed from the identified library elements.

10. The method of claim 1, wherein:

one or more of the sources have type information representing a role played by the source in a chemical reaction and equivalence information quantifying behavior relating to the role; and

one or more of the maps define amounts for the one or more sources based in part on the equivalence information.

11. A computer program product on a computer-readable medium for generating a library design for a set of experiments, comprising instructions operable to cause a programmable processor to:

define a library array representing an arrangement of experiments in the set of experiments, the library array including electronic data defining a plurality of elements, each of the plurality of elements representing a potential location for an experiment in the set of experiments;

define a plurality of sources, each of the plurality of sources including electronic data representing a material or condition that can be used in the set of experiments;

receive user input defining a plurality of maps representing the application of sources to elements of the library array, each of the plurality of maps including electronic data identifying one or more library elements and defining an amount of a corresponding source to be applied to the identified library elements, the plurality of maps being ordered to define a mapping sequence; and

generate a library design including electronic data representing the library array, the sources, the maps and the mapping sequence, the library design specifying for each of a plurality of library elements amounts of one or more sources to be applied to the corresponding library element, the amounts being defined at least in part by the order of maps in the mapping sequence.

12. The computer program product of claim 11, further comprising instructions operable to cause a programmable processor to:

display a visual representation of a plurality of experiments in the set of experiments.

13. The computer program product of claim 12, wherein:
the visual representation includes a representation of at least a portion of a
composition including the specified amounts for a plurality of library elements corresponding
5 to the plurality of experiments.

14. The computer program product of claim 12, wherein:
the visual representation includes a representation of the mapping sequence, the maps
in the mapping sequence being selectable in the visual representation.

15. The computer program product of claim 14, wherein:
the visual representation includes a representation of a portion of a composition
including the specified amounts for a plurality of library elements, the portion being
determined based on a set of maps selected by the user.

16. The computer program product of claim 11, wherein:
one or more of the maps in the mapping sequence has an associated equation defining
a mathematical relationship for determining the amount of the corresponding source to be
applied to the identified library elements based on an amount defined by a prior map in the
20 mapping sequence.

17. The computer program product of claim 16, wherein:
the mapping sequence includes a first group of maps, the first group of maps having a
first set of associated equations defining a plurality of mathematical relationships for
25 determining the amount of one or more sources to be applied to one or more identified library
elements, the first set of associated equations being solvable as a set of simultaneous
equations.

18. The computer program product of claim 17, wherein:
the mapping sequence includes a second group of maps, the second group of maps
30 having a second set of associated equations defining a plurality of mathematical relationships

for determining the amount of one or more sources to be applied to one or more identified library elements, the first set of associated equations and second set of associated equations being separately solvable as sets of simultaneous equations.

5 19. The computer program product of claim 11, wherein:

the plurality of maps includes a remove map defining an amount of a source to be removed from the identified library elements.

20. The computer program product of claim 11, wherein:

10 one or more of the sources have type information representing a role played by the source in a chemical reaction and equivalence information quantifying behavior relating to the role; and

one or more of the maps define amounts for the one or more sources based in part on the equivalence information.

15 21. The method of claim 1, wherein:

one or more sources of the plurality of sources include electronic data representing a mixture of chemicals to be used in the set of experiments, the one or more sources including type information representing the one or more sources as including one or more chemicals in the mixture of chemicals and equivalence information representing an amount of the one or more chemicals included in the mixture of chemicals; and

the library design specifies amounts of the one or more chemicals in the mixture of chemicals to be applied to one or more of the library elements, the specified amounts being determined based on the type information and the equivalence information for the one or more sources.

22. The computer program product of claim 11, wherein:

one or more sources of the plurality of sources include electronic data representing a mixture of chemicals to be used in the set of experiments, the one or more sources including type information representing the one or more sources as including one or more chemicals in

the mixture of chemicals and equivalence information representing an amount of the one or more chemicals included in the mixture of chemicals; and

the library design specifies amounts of the one or more chemicals in the mixture of chemicals to be applied to one or more of the library elements, the specified amounts being

5 determined based on the type information and the equivalence information for the one or more sources.